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A free-energy surface exploration algorithm for supercooled liquids and amorphous solids KIRK D. LEWIS, YONGWOO SHIN, XI LIN, Boston University, BU TEAM — Efficient exploration of the multidimensional free-energy surfaces (FES) of supercooled liquids and amorphous solids at low temperatures is extremely challenging. The recently developed autonomous basin-climbing (ABC) algorithm (JCP 130: 224504, 2009) allows the sluggish system to self-explore the multidimensional potential energy surface (PES) and climb out of deep energy basins through a series of collective activation and relaxation events. In this work, we present a new FES exploration algorithm that enforces an explicit temperature dependence on the ABC trajectories. The explicit temperature dependence is achieved by introducing an ensemble of walkers to collectively maintain the detailed balance criteria among all the relevant energy basins. Using this new algorithm, the metabasin correlation length of a binary Lennard-Jones supercooled liquid is identified at the glass transition temperature.

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